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Pressure Dependence of Atomic Structure, Magnetism, and Elastic Properties of Fe₃C: a Combined Synchrotron X-ray Diffraction and Nuclear Resonant Scattering Study

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In this work, we demonstrate the feasibility of studying atomic structure, magnetism, and elastic properties with combined synchrotron x-ray diffraction (XRD) and nuclear resonant scattering methods on Fe₃C at beamlines 3-ID, 11-BM, 13-BM, and 13-ID at the Advanced Photon Source. XRD probes the long-range order of a material and is a classic method for measuring density. From density-versus-pressure data, elastic properties such as bulk modulus and its pressure derivative can be derived from equation-of-state (EoS) fitting. For EoS fitting, we developed a Java program, FitEoS, which is available to the public. Nuclear resonant scattering technique includes synchrotron Mössbauer spectroscopy and nuclear resonant inelastic x-ray scattering methods. These methods provide information on magnetic properties and lattice vibration. A combination of these methods provides a unique understanding on the behavior of a material under pressure from various perspectives. In this study, we observed two discontinuities in the XRD compression data on Fe₃C. These two discontinuities were suggested to be related to magnetic and electronic transitions from our nuclear resonant scattering measurements. The implications about the Earth's inner core inferred from this work will also be discussed.

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